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                 and PCTGEN
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         JUL 19
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                 databases provides new, more efficient competitor
                 analyses
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         JUL 26
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                 MEDLINE Cited References provide additional
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                 revelant records with no additional searching.
NEWS 20
         OCT 04
                 Removal of Pre-IPC 8 data fields streamlines
                 displays in USPATFULL, USPAT2, and USPATOLD.
NEWS 21
         OCT 04
                 Precision of EMBASE searching enhanced with new
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NEWS 22 OCT 06
                 Increase your retrieval consistency with new formats
                 for Taiwanese application numbers in CA/CAplus.
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- NEWS 25 OCT 28 INPADOCDB/INPAFAMDB: Enhancements to the US national patent classification.
- NEWS 26 NOV 03 New format for Korean patent application numbers in CA/CAplus increases consistency, saves time.

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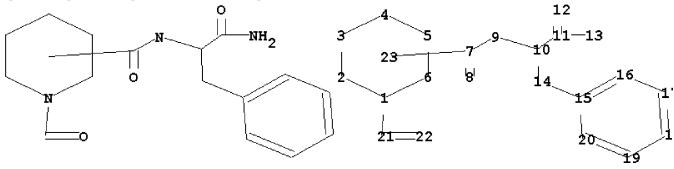
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chain nodes :

7 8 9 10 11 12 13 14 21 22 24 25 26 27

ring nodes :

1 2 3 4 5 6 15 16 17 18 19 20

chain bonds :

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 15-16 \quad 15-20 \quad 16-17 \quad 17-18 \quad 18-19 \quad 19-20$ 

exact/norm bonds :

 $1-2 \quad 1-6 \quad 1-21 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-9 \quad 9-10 \quad 11-12 \quad 11-13 \quad 21-22$ 

exact bonds :

10-11 10-14 14-15

normalized bonds :

 $15-16 \quad 15-20 \quad 16-17 \quad 17-18 \quad 18-19 \quad 19-20 \quad 24-25 \quad 24-26 \quad 24-27$ 

isolated ring systems :

containing 1 :

## Match level:

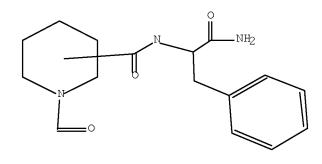
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## L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 298 TO ITERATE

100.0% PROCESSED 298 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 4925 TO 6995 PROJECTED ANSWERS: 2 TO 124

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FULL SCREEN SEARCH COMPLETED - 5877 TO ITERATE

100.0% PROCESSED 5877 ITERATIONS 121 ANSWERS

SEARCH TIME: 00.00.01

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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN

GΙ

The invention relates to phosphonic acid derivs. R1-X1-P(0) (X2-R2)-Y-Z-W1(A1-R3) (A2-R4)-W2(A3-R5) (A4-R6)-W3(A5-R7) (A6-R8)- A7-Q(T)-V(U)-A8-CR9R10-A9-R11 [R1, R2 are independently H or phospho-protecting groups; X1, X2 are independently O, S or NR12; Z is O, S, NR13 or CR4R5; A1-A9 are independently null, O, S, NR16, SO, SO2, CO, C(S), NR17CO, NR18C(S), NR19CONR2O, NR21C(S)NR22, NR23S(O), NR24SO2 or NR25CO2; Y is O or CR26R27; Q, V are independently CR28 or N; W1, W2, W3 are independently C or N; R3-R28, T, U are independently null, H, halo, (un)substituted alkyl, cycloalkyl, heterocyclyl, aryl, heteroaryl, etc.; or T and U may be connected by a single or double bond] and to pharmaceutical compns. containing the compds. for the treatment of diseases involving abnormal or undesired cell proliferation or mitosis. Thus, peptide phosphonic acid derivative I, prepared via peptide coupling in the solid phase, was a potent rotamase inhibitor (IC50 < 1  $\mu$ M).

AN 2005:612099 CAPLUS Full-text

DN 143:133696

TI Preparation of peptide phosphonic acid derivatives for the inhibition of undesired cell proliferation

IN Knolle, Jochen; Schutkowski, Mike; Hummel, Gerd; Tradler, Thomas; Jobron, Laurence; Christner, Claudia; Gibson, Christoph; Zischinsky, Gunther

PA Jerini A.-G., Germany

SO PCT Int. Appl., 110 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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    (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
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(Uses)

WO 2004-EP14460

W 20041218

(preparation of peptide phosphonic acid derivs. for inhibition of undesired cell proliferation)

RN 858352-55-3 CAPLUS

CN L-Alaninamide, N-acetyl-3-benzo[b]thien-3-yl-L-alanyl-O-(phosphonomethyl)-L-seryl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-56-4 CAPLUS

CN L-Alaninamide, N-acetyl-3-benzo[b]thien-3-yl-L-alanyl-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-57-5 CAPLUS

CN L-Alaninamide, N-acetyl-3-benzo[b]thien-3-yl-L-alanyl-S-(phosphonomethyl)-D-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-58-6 CAPLUS

CN L-Alaninamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-O-(phosphonomethyl)-L-

Absolute stereochemistry.

RN 858352-59-7 CAPLUS

CN L-Alaninamide, N-[3-[[(4-chlorophenyl)methyl]thio]-1-oxopropyl]-S- (phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-60-0 CAPLUS

CN L-Alaninamide, N-[3-[[(3,4-dichlorophenyl)methyl]thio]-1-oxopropyl]-S- (phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

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RN 858352-61-1 CAPLUS

CN L-Alaninamide, N-[5-(4-chlorophenyl)-1,5-dioxopentyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-62-2 CAPLUS

CN L-Alaninamide, N-(1-oxo-5-phenylpentyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-63-3 CAPLUS

CN L-Alaninamide, 3-benzo[b]thien-3-yl-N-[6-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)amino]thioxomethyl]amino]-1-oxohexyl]-L-alanyl-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 858352-64-4 CAPLUS

CN L-Alaninamide, N-[(2,5-dioxo-4-imidazolidinyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-65-5 CAPLUS

CN L-Alaninamide, N-(cyclohexylacetyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858352-66-6 CAPLUS

CN L-Alaninamide, 2-oxo-4-thiazolidinecarbonyl-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-67-7 CAPLUS

CN L-Alaninamide, 2-oxo-4-thiazolidinecarbonyl-2-oxo-4-thiazolidinecarbonyl-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-68-8 CAPLUS

CN L-Alaninamide, N-(3-phenoxybenzoyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858352-69-9 CAPLUS

CN L-Alaninamide, S-(phosphonomethyl)-N-[(1,2,3,4-tetrahydro-2-naphthalenyl)carbonyl]-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-70-2 CAPLUS

CN L-Alaninamide, N-[1-oxo-3-(2-thienyl)propyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-71-3 CAPLUS

CN L-Alaninamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858352-72-4 CAPLUS

CN L-Alaninamide, 3-benzo[b]thien-3-yl-N-(4-piperidinylcarbonyl)-L-alanyl-S- (phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-73-5 CAPLUS

CN L-Alaninamide, 3-benzo[b]thien-3-yl-N-(1-piperazinylacetyl)-L-alanyl-S- (phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

CN L-Alaninamide, N-benzoyl-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-75-7 CAPLUS

CN L-Alaninamide, N-(phenylacetyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-76-8 CAPLUS

CN L-Alaninamide, N-(1-oxo-3-phenylpropyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-77-9 CAPLUS

CN L-Alaninamide, N-(1-oxo-4-phenylbutyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858352-78-0 CAPLUS

CN L-Alaninamide, N-([1,1'-biphenyl]-4-ylacetyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-82-6 CAPLUS

CN Phosphonic acid, [[[2-[(2S)-2-[[[(1S)-2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-2-oxoethyl]thio]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-83-7 CAPLUS

CN Phosphonic acid, [[[3-[(2S)-2-[[[(1S)-2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-3-oxopropyl]thio]methyl]- (9CI) (CA INDEX NAME)

RN 858352-84-8 CAPLUS

CN L-Alaninamide, N-acetyl-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-85-9 CAPLUS

CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-86-0 CAPLUS

CN L-Alaninamide, N-[(phenylmethyl)sulfonyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858352-87-1 CAPLUS

CN L-Alaninamide, N-[(1-phenylcyclopentyl)carbonyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-88-2 CAPLUS

CN L-Alaninamide, N-[(2-chlorophenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl- (2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-89-3 CAPLUS

CN L-Alaninamide, N-[(4-chlorophenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl- (2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858352-90-6 CAPLUS

CN L-Alaninamide, N-[(4-methoxyphenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-91-7 CAPLUS

CN L-Alaninamide, N-[4-(4-chlorophenyl)-1,4-dioxobutyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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RN 858352-92-8 CAPLUS

CN L-Alaninamide, N-[4-(4-methoxyphenyl)-1-oxobutyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858352-93-9 CAPLUS

CN L-Alaninamide, 5-oxo-L-prolyl-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-94-0 CAPLUS

CN L-Alaninamide, N-(3-benzofuranylcarbonyl)-S-(phosphonomethyl)-L-cysteinyl- (2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-95-1 CAPLUS

CN L-Alaninamide, S-(phosphonomethyl)-N-(1-piperazinylacetyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858352-96-2 CAPLUS

CN L-Alaninamide, (4R)-3-acetyl-2-oxo-4-thiazolidinecarbonyl-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-97-3 CAPLUS

CN L-Alaninamide, N-[(2-methylpropoxy)carbonyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858352-98-4 CAPLUS

CN L-Alaninamide, N-(butoxycarbonyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858352-99-5 CAPLUS

CN L-Alaninamide, N-(methoxycarbonyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-00-1 CAPLUS

CN L-Alaninamide, N-(phenoxycarbonyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-01-2 CAPLUS

CN L-Alaninamide, N-[(2-phenylethoxy)carbonyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-02-3 CAPLUS

CN L-Alaninamide, N-(phenylsulfonyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-03-4 CAPLUS

CN L-Alaninamide, N-[(2-phenylethyl)sulfonyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-04-5 CAPLUS

CN L-Alaninamide, N-[(3-phenylpropyl)sulfonyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-05-6 CAPLUS

CN L-Alaninamide, N-(methylsulfonyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-06-7 CAPLUS

CN L-Alaninamide, S-(phosphonomethyl)-N-[(2,4,6-trimethylphenyl)sulfonyl]-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-07-8 CAPLUS

CN L-Alaninamide, S-(phosphonomethyl)-N-(2-thienylsulfonyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-08-9 CAPLUS

CN L-Alaninamide, N-[1-oxo-3-(1-piperidinyl)propyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-10-3 CAPLUS

CN L-Alaninamide, N-(1,3-benzodioxol-5-ylacetyl)-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-11-4 CAPLUS

CN L-Alaninamide, N-[(3,5-dimethoxyphenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-12-5 CAPLUS

CN L-Alaninamide, N-[(2-methoxyphenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl- (2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-15-8 CAPLUS

CN L-Alaninamide, N-[(3-methoxyphenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl- (2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-16-9 CAPLUS

CN L-Alaninamide, S-(phosphonomethyl)-N-[[4-(1-piperazinyl)phenyl]acetyl]-L-cysteinyl-(2S)-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-19-2 CAPLUS

CN Phosphonic acid, [[[2-[(2S)-2-[[[(1S)-2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-1-methyl-2-oxoethyl]thio]methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-23-8 CAPLUS

CN Phosphonic acid, [[[1-[[(2S)-2-[[[(1S)-2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]carbonyl]-3-(methylamino)-3-oxopropyl]thio]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-24-9 CAPLUS

CN Phosphonic acid, [[[1-[[(2S)-2-[[[(1S)-2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]carbonyl]-3-[(4-methoxyphenyl)amino]-3-oxopropyl]thio]methyl]- (9CI) (CA INDEX NAME)

RN 858353-52-3 CAPLUS

CN Alaninamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-O-(phosphonomethyl)-L-seryl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2N$$
 $H_2N$ 
 $H_3N$ 
 $H_4N$ 
 $H_4N$ 

RN 858353-53-4 CAPLUS

CN Alaninamide, N-[3-[[(4-chlorophenyl)methyl]thio]-1-oxopropyl]-S- (phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-54-5 CAPLUS

CN Alaninamide, N-[3-[[(3,4-dichlorophenyl)methyl]thio]-1-oxopropyl]-S- (phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{C1} \\ \\ \text{S} \\ \\ \text{H}_{2}\text{N} \\ \\ \text{O} \\ \\ \text{PO}_{3}\text{H}_{2} \\ \\ \text{O} \\ \\ \text$$

RN 858353-55-6 CAPLUS

CN Alaninamide, N-[5-(4-chlorophenyl)-1,5-dioxopentyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-56-7 CAPLUS

CN Alaninamide, N-(1-oxo-5-phenylpentyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-57-8 CAPLUS

CN Alaninamide, N-(cyclohexylacetyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-58-9 CAPLUS

CN Alaninamide, N-(3-phenoxybenzoyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-59-0 CAPLUS

CN Alaninamide, N-[1-oxo-3-(2-thienyl)propyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-60-3 CAPLUS

CN Alaninamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-61-4 CAPLUS

CN Alaninamide, N-benzoyl-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-62-5 CAPLUS

CN Alaninamide, N-(phenylacetyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-63-6 CAPLUS

CN Alaninamide, N-(1-oxo-3-phenylpropyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-64-7 CAPLUS

CN Alaninamide, N-(1-oxo-4-phenylbutyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-65-8 CAPLUS

CN Alaninamide, N-([1,1'-biphenyl]-4-ylacetyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} H & R & S & PO3H2 \\ \hline \\ Ph & H_2N & O & \\ \end{array}$$

RN 858353-69-2 CAPLUS

CN Phosphonic acid, [[[2-[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-2-oxoethyl]thio]methyl]- (9CI) (CA INDEX NAME)

RN 858353-70-5 CAPLUS

CN Phosphonic acid, [[[3-[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-3-oxopropyl]thio]methyl]- (9CI) (CA INDEX NAME)

RN 858353-71-6 CAPLUS

CN Alaninamide, N-acetyl-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-72-7 CAPLUS

CN Alaninamide, N-[(phenylmethoxy)carbonyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-73-8 CAPLUS

CN Alaninamide, N-[(phenylmethyl)sulfonyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-74-9 CAPLUS

CN Alaninamide, N-[(1-phenylcyclopentyl)carbonyl]-S-(phosphonomethyl)-Lcysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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RN 858353-75-0 CAPLUS

CN Alaninamide, N-[(2-chlorophenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-76-1 CAPLUS

CN Alaninamide, N-[(4-chlorophenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-77-2 CAPLUS

CN Alaninamide, N-[(4-methoxyphenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} H \\ N \\ R \\ N \\ N \end{array}$$

RN 858353-78-3 CAPLUS

CN Alaninamide, N-[4-(4-chlorophenyl)-1,4-dioxobutyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

$$C1$$
 $R$ 
 $R$ 
 $S$ 
 $PO3H2$ 
 $H_2N$ 
 $O$ 

RN 858353-79-4 CAPLUS

CN Alaninamide, N-[4-(4-methoxyphenyl)-1-oxobutyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-80-7 CAPLUS

CN Alaninamide, 5-oxo-L-prolyl-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-81-8 CAPLUS

CN Alaninamide, N-(3-benzofuranylcarbonyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-82-9 CAPLUS

CN Alaninamide, S-(phosphonomethyl)-N-(1-piperazinylacetyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 858353-83-0 CAPLUS

CN Alaninamide, N-[(2-methylpropoxy)carbonyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-84-1 CAPLUS

CN Alaninamide, N-(butoxycarbonyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-85-2 CAPLUS

CN Alaninamide, N-(methoxycarbonyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-86-3 CAPLUS

CN Alaninamide, N-(phenoxycarbonyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-87-4 CAPLUS

CN Alaninamide, N-[(2-phenylethoxy)carbonyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-88-5 CAPLUS

CN Alaninamide, N-(phenylsulfonyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-89-6 CAPLUS

CN Alaninamide, N-[(2-phenylethyl)sulfonyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-90-9 CAPLUS

CN Alaninamide, N-[(3-phenylpropyl)sulfonyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-91-0 CAPLUS

CN Alaninamide, N-(methylsulfonyl)-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-92-1 CAPLUS

CN Alaninamide, S-(phosphonomethyl)-N-[(2,4,6-trimethylphenyl)sulfonyl]-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-93-2 CAPLUS

CN Alaninamide, S-(phosphonomethyl)-N-(2-thienylsulfonyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-94-3 CAPLUS

CN Alaninamide, N-[1-oxo-3-(1-piperidinyl)propyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858353-96-5 CAPLUS

CN Alaninamide, N-(1,3-benzodioxol-5-ylacetyl)-S-(phosphonomethyl)-Lcysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 858353-97-6 CAPLUS

CN Alaninamide, N-[(3,5-dimethoxyphenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858353-98-7 CAPLUS

CN Alaninamide, N-[(2-methoxyphenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{OMe} \\ \text{H} \\ \text{N} \\ \text{R} \\ \text{S} \\ \text{PO}_{3}\text{H}_{2} \\ \text{O} \\ \text$$

RN 858354-02-6 CAPLUS

CN Alaninamide, N-[(3-methoxyphenyl)acetyl]-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858354-03-7 CAPLUS

CN Alaninamide, S-(phosphonomethyl)-N-[[4-(1-piperazinyl)phenyl]acetyl]-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 858354-06-0 CAPLUS

CN Phosphonic acid, [[[2-[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-1-methyl-2-oxoethyl]thio]methyl]-(9CI) (CA INDEX NAME)

RN 858354-10-6 CAPLUS

CN Phosphonic acid, [[[1-[[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]carbonyl]-3-(methylamino)-3-oxopropyl]thio]methyl]- (9CI) (CA INDEX NAME)

RN 858354-11-7 CAPLUS

CN Phosphonic acid, [[[1-[[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]carbonyl]-3-[(4-methoxyphenyl)amino]-3-oxopropyl]thio]methyl]- (9CI) (CA INDEX NAME)

RN 858648-21-2 CAPLUS

CN Alaninamide, N-acetyl-3-benzo[b]thien-3-ylalanyl-0-(phosphonomethyl)-L-seryl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858648-22-3 CAPLUS

CN Alaninamide, N-acetyl-3-benzo[b]thien-3-ylalanyl-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858648-23-4 CAPLUS

CN Alaninamide, 3-benzo[b]thien-3-yl-N-[6-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)amino]thioxomethyl]amino]-1-oxohexyl]alanyl-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

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PAGE 1-B

RN 858648-24-5 CAPLUS

CN Phosphonic acid, [[[(2R)-3-[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-2-[[(2,5-dioxo-4-imidazolidinyl)acetyl]amino]-3-oxopropyl]thio]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & &$$

RN 858648-25-6 CAPLUS

CN Phosphonic acid, [[[(2R)-3-[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-3-oxo-2-[[(2-oxo-4-thiazolidinyl)carbonyl]amino]propyl]thio]methyl]- (9CI) (CA INDEX NAME)

RN 858648-26-7 CAPLUS

CN Phosphonic acid, [[[(2R)-3-[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-3-oxo-2-[[[2-oxo-3-[(2-oxo-4-thiazolidinyl)carbonyl]-4-thiazolidinyl]carbonyl]amino]propyl]thio]methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858648-27-8 CAPLUS

CN Phosphonic acid, [[[(2R)-3-[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-3-oxo-2-[[(1,2,3,4-tetrahydro-2-naphthalenyl)carbonyl]amino]propyl]thio]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 858648-28-9 CAPLUS

CN Alaninamide, 3-benzo[b]thien-3-yl-N-(4-piperidinylcarbonyl)alanyl-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)-(9CI) (CA INDEX NAME)

RN 858648-29-0 CAPLUS

CN Alaninamide, 3-benzo[b]thien-3-yl-N-(1-piperazinylacetyl)alanyl-S-(phosphonomethyl)-L-cysteinyl-2-piperidinecarbonyl-3-(2-naphthalenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 858648-30-3 CAPLUS

CN Phosphonic acid, [[[(2R)-2-[[(3-acetyl-2-oxo-4-thiazolidinyl)carbonyl]amino]-3-[2-[[[2-amino-1-(2-naphthalenylmethyl)-2-oxoethyl]amino]carbonyl]-1-piperidinyl]-3-oxopropyl]thio]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 858353-37-4DP, resin-bound

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of peptide phosphonic acid derivs. for inhibition of undesired

cell proliferation)

RN 858353-37-4 CAPLUS

CN L-Alaninamide, S-(phosphonomethyl)-L-cysteinyl-(2S)-2-piperidinecarbonyl-3- (2-naphthalenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> file registry

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 15.81 207.57

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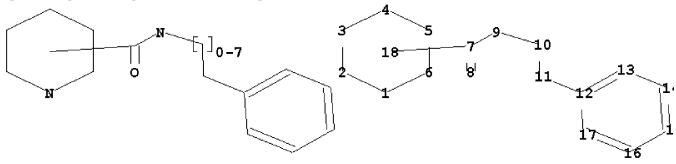
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20

22

21



chain nodes :

7 8 9 10 11 19 20 21 22

ring nodes :

1 2 3 4 5 6 12 13 14 15 16 17

chain bonds :

7-8 7-9 9-10 10-11 11-12 19-20 19-21 19-22

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16 \quad 16-17$ 

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-9 9-10

exact bonds :

10-11 11-12

normalized bonds :

 $12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16 \quad 16-17 \quad 19-20 \quad 19-21 \quad 19-22$ 

isolated ring systems :

containing 1:

## Match level :

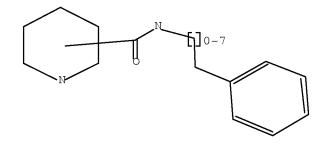
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS

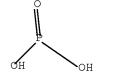
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L5 HAS NO ANSWERS

L5 STR





Structure attributes must be viewed using STN Express query preparation.

=> s 15

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SAMPLE SCREEN SEARCH COMPLETED - 189 TO ITERATE

100.0% PROCESSED 189 ITERATIONS 7 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2956 TO 4604

PROJECTED ANSWERS: 7 TO 298

L6 7 SEA SSS SAM L5

=> s 15

SAMPLE SEARCH INITIATED 15:52:22 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 189 TO ITERATE

100.0% PROCESSED 189 ITERATIONS 7 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2956 TO 4604 PROJECTED ANSWERS: 7 TO 298

L7 7 SEA SSS SAM L5

=> ful

FUL IS NOT A RECOGNIZED COMMAND

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=> s 15 ful

FULL SEARCH INITIATED 15:52:31 FILE 'REGISTRY'

100.0% PROCESSED 3948 ITERATIONS

SEARCH TIME: 00.00.01

L8 211 SEA SSS FUL L5

=> d his

(FILE 'HOME' ENTERED AT 15:38:31 ON 03 NOV 2010)

211 ANSWERS

FILE 'REGISTRY' ENTERED AT 15:38:58 ON 03 NOV 2010

STRUCTURE UPLOADED L1

L2 2 S L1

T.3 121 S L1 FUL

FILE 'CAPLUS' ENTERED AT 15:39:37 ON 03 NOV 2010

L41 S L3

FILE 'REGISTRY' ENTERED AT 15:51:42 ON 03 NOV 2010

L5 STRUCTURE UPLOADED

7 S L5 L6 L7 7 S L5

L8 211 S L5 FUL

=> s 18 not 13

90 L8 NOT L3

=> file caplus

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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=> s 19 L10 33 L9

=> d abs bib fhitstr 25-33

L10 ANSWER 25 OF 33 CAPLUS COPYRIGHT 2010 ACS on STN

AB The author used photolytic liberation of either caged isocitrate or caged NADP and Laue X-ray data collection to visualize the isocitrate dehydrogenase complex. The experiment was conducted with three different photoreactive compds., each possessing a unique mechanism leading to the formation of the ES complex. Photoreaction efficiency and subsequent substrate affinities and binding rates in the crystal are critical parameters in these expts.

AN 1999:142636 CAPLUS Full-text

DN 130:348950

TI Visualization enzyme intermediates using fast diffraction and reaction trapping methods isocitrate dehydrogenase

AU Stoddard, B. L.

CS Div. Basic Sciences, Fred Hutchinson Cancer Res. Center, Seattle, WA, 98109, USA

SO Biochemical Society Transactions (1999), 27(2), 42-48 CODEN: BCSTB5; ISSN: 0300-5127

PB Portland Press Ltd.

DT Journal

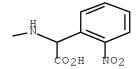
LA English

IT 193008-54-7

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process) (photoreactive substrates; visualizing isocitrate dehydrogenase intermediates using fast X-ray diffraction and reaction trapping methods)

RN 193008-54-7 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate), 2'-(dihydrogen phosphate),  $P' \rightarrow 5'$ -ester with 3-[[[carboxy(2-nitrophenyl)methyl]amino]carbonyl]-1- $\beta$ -D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)



OSC.G 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 26 OF 33 CAPLUS COPYRIGHT 2010 ACS on STN

AB The structure of a rate-limited product complex formed during a single initial round of turnover by isocitrate dehydrogenase has been determined Photolytic liberation of either caged substrate or caged cofactor and Laue X-ray data collection were used to visualize the complex, which has a min. half-life of approx. 10 ms. The experiment was conducted with three different photoreactive compds., each possessing a unique mechanism leading to the formation of the enzyme-substrate (ES) complex. Photoreaction efficiency and subsequent substrate affinities and binding rates in the crystal are critical parameters for these expts. The structure suggests that CO2 dissociation is a rapid event that may help drive product formation, and that small conformational changes may contribute to slow product release.

AN 1998:699517 CAPLUS Full-text

DN 130:49120

TI Millisecond Laue structures of an enzyme-product complex using photocaged substrate analogs

AU Stoddard, Barry L.; Cohen, Bruce E.; Brubaker, Michael; Mesecar, Andrew D.; Koshland, Daniel E., Jr.

CS Division of Basic Sciences, Program in Structural Biology, Fred Hutchinson Cancer Research Center A3-023, Seattle, WA, 98109, USA

SO Nature Structural Biology (1998), 5(10), 891-897 CODEN: NSBIEW; ISSN: 1072-8368

PB Nature America

DT Journal

LA English

IT 193008-54-7

RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(caged substrate analog; millisecond Laue structures of an enzyme-product complex using photocaged substrate analogs)

RN 193008-54-7 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate), 2'-(dihydrogen phosphate),  $P' \rightarrow 5'$ -ester with 3-[[carboxy(2-nitrophenyl)methyl]amino]carbonyl]-1- $\beta$ -D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

PAGE 1-B

OSC.G 25 THERE ARE 25 CAPLUS RECORDS THAT CITE THIS RECORD (25 CITINGS)

RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 27 OF 33 CAPLUS COPYRIGHT 2010 ACS on STN

AΒ Two caged NADP compds. have been synthesized and characterized for use in the crystallog. study of isocitrate dehydrogenase (IDH), as well as for general use in cell biol., metabolism, and enzymol. One caged NADP compound has been designed to be "catalytically caged" so that it can bind to IDH prior to photolysis but is not catalytically active. A second NADP compound is "affinity caged" so that addition of the caging group inhibits binding of the compound to IDH prior to photolysis. The catalytically caged compound was synthesized in a two-step process, starting with the NADase-catalyzed exchange of a synthetic nicotinamide derivative onto NADP. X-ray structures of the NADP compds. with IDH show the catalytically caged NADP bound to the enzyme with its nicotinamide group improperly positioned to allow turnover, while the affinity caged NADP does not bind to the enzyme at concns. up to 50 mM. Two analogous caged NAD compds. have also been synthesized. The NADP and NAD compds. were characterized in terms of kinetics, quantum yield, and product formation. The affinity caged NADP compound P2'-[1-(4,5-dimethoxy-2nitrophenyl)ethyl] NADP is photolyzed at a rate of 1.8+104 s-1 with a quantum yield of 0.19 at pH 7; the NAD analog P-[1-(4,5-dimethoxy-2-nitrophenyl)ethyl] NAD is photolyzed at a rate of 1.7+104 s-1 with a quantum yield of 0.17.

AN 1997:425310 CAPLUS Full-text

DN 127:132644

OREF 127:25517a,25520a

TI Caged NADP and NAD. Synthesis and Characterization of Functionally Distinct Caged Compounds

AU Cohen, Bruce E.; Stoddard, Barry L.; Koshland, Daniel E., Jr.

CS Departments of Chemistry and Molecular and Cell Biology, University of California, Berkeley, CA, 94720-3206, USA

SO Biochemistry (1997), 36(29), 9035-9044 CODEN: BICHAW; ISSN: 0006-2960

PB American Chemical Society

DT Journal

LA English

OS CASREACT 127:132644

IT 193008-54-7P

RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent) (synthesis and photochem. characterization of caged NADP and NAD compds. for use in Laue crystallog. study of isocitrate dehydrogenase)

RN 193008-54-7 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate), 2'-(dihydrogen phosphate),  $P' \rightarrow 5'$ -ester with 3-[[carboxy(2-nitrophenyl)methyl]amino]carbonyl]-1- $\beta$ -D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

OSC.G 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)

L10 ANSWER 28 OF 33 CAPLUS COPYRIGHT 2010 ACS on STN

AB Peptides X-PTI-(AA)n-Y (AA = natural or unnatural amino acid residue, n = 0-15, PTI = tyrosine or preferably phosphotyrosine or phosphotyrosine mimic, X = arylcarbonyl, cycloalkylcarbonyl, tricycloalkylcarbonyl, arylsulfonyl, etc., Y = OH, C-terminal protecting group, amino group) or their salts were prepared for the treatment of diseases that respond to inhibition of the interaction of a protein comprising an SH2 domain and a protein tyrosine. Thus, 3-aminobenzyloxycarbonyl-Tyr(PO3H2)-Ile-Asn-Gln-NH2 trifluoroacetate salt was prepared by the solid phase method and had an IC50 value of 0.1 in a test system using the phosphorylated "tail" EGFR-MBP fusion protein as ligand. Formulations containing acylated oligopeptides are described.

AN 1997:283758 CAPLUS Full-text

DN 126:264364

OREF 126:51209a,51212a

TI Acylated oligopeptide derivatives having cell signal inhibiting activity

IN Garcia-Echeverria, Carlos; Gay, Brigitte; Furet, Pascal; Rahuel, Joseph;
Caravatti, Giorgio; Fretz, Heinz; Schoepfer, Joseph

PA Ciba-Geigy A.-G., Switz.

SO PCT Int. Appl., 257 pp. CODEN: PIXXD2

DT Patent

#### LA English

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FAN.	CNT	1

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	WO	1996	-EP3	473		W		1996	0806										
OS	MAF	RPAT	126:	2643	64														

188749-84-0P ΙT

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of acylated oligopeptide derivs. having cell signal inhibiting activity)

RN 188749-84-0 CAPLUS

L-Glutamamide, O-phosphono-N-(4-pyridinylcarbonyl)-L-tyrosyl-L-isoleucyl-L-CN asparaginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

OSC.G THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 29 OF 33 CAPLUS COPYRIGHT 2010 ACS on STN

AB The synthesis of caged NAD+ and caged NADP+ coenzymes was achieved by using pig brain NADase to exchange nicotinamide with N-2-nitrobenzylnicotinamide. The synthesis of N-2 nitrobenzylnicotinamide is achieved by the coupling of onitrobenzyl amine with nicotinoyl chloride. The photorelease of NADP+ is characterized and the quantum efficiency of NADP+ release measured. The biol. inactivity of caged NADP+ is established for several dehydrogenases and the biol. activity of released NADP+ demonstrated.

AN 1997:196181 CAPLUS Full-text

DN 126:289866

OREF 126:56033a,56036a

TI Synthesis of Caged NAD(P) + Coenzymes: Photorelease of NADP+

AU Salerno, Charles P.; Resat, Marianne; Magde, Douglas; Kraut, Joseph

CS Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA, 92093-0506, USA

SO Journal of the American Chemical Society (1997), 119(14), 3403-3404 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

IT 189169-98-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative)

(synthesis of caged NAD(P) + coenzymes)

RN 189169-98-0 CAPLUS

CN Adenosine 5'-(trihydrogen diphosphate), 2'-(dihydrogen phosphate),  $P' \rightarrow 5'$ -ester with 3-[[(2-nitrophenyl)methyl]amino]carbonyl]-1-  $\beta$ -D-ribofuranosylpyridinium, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

OSC.G 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

AΒ Title compds., conjugates comprising a 1st residue and a 2nd residue connected by a cleavable bond, wherein the 1st residue is an inhibitor of the biosynthesis of an adrenergic neurotransmitter and the 2nd residue is cleaved by an enzyme located predominantly in the kidney, are prepared 5-[(5-Butyl-2pyridinyl)carbonyl]-L-glutamic acid hydrazide (preparation given) in MeCN/H2O was treated with 2 equiv of 1M K2CO3 followed by Ac2O and K2CO3 to give the Lglutamic hydrazide I. In spontaneously hypertensive rats, I at 8 mg/h lowered blood pressure from 146 to 122 mm Hg on day 1 and to 115 mm Hg on day 5. Addnl. compds. were prepared and tested. A large number of compds. are claimed.

1991:583950 CAPLUS Full-text ΑN

DN 115:183950

OREF 115:31445a,31448a

Preparation of amino acid conjugates as renal-selective prodrugs for the TΤ treatment of hypertension

Reitz, David B.; Koepke, John P.; Blaine, Edward H.; Schuh, Joseph R.; ΙN Manning, Robert E.; Smits, Glenn J.

G.D. Searle and Co., USA PA

PCT Int. Appl., 459 pp. CODEN: PIXXD2

Patent DT

English

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	US	1994	-280	170		В1		1994	0725								
	US	1996	-639	493		В1		1996	0429								
	US	1999	-4448	888		В1		1999	1122								
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ΙT 136486-36-7DP, kidney enzyme-cleavable conjugate

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as prodrug antihypertensive)

136486-36-7 CAPLUS RN

CN L-Tyrosine, 3-hydroxy-N-[[5-(hydroxymethyl)-2-methyl-3-(phosphonooxy)-4Absolute stereochemistry.

OSC.G 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 31 OF 33 CAPLUS COPYRIGHT 2010 ACS on STN

The coenzyme-amino acid adducts, N-(5'-phosphopyridoxyl)-L-3,4-AB dihydroxyphenylalanine and N-(5'-phosphopyridoxyl)-L-m-aminotyrosine (I),inhibit hog kidney aromatic L-amino acid decarboxylase (DOPA decarboxylase, II). Kinetic studies on the nature of the inhibition caused by these adducts appeared to distinguish 2 distinct decarboxylase activities in purified enzyme prepns. The appearance of 2 activities in purified enzyme prepns. is an artifact of the system resulting from the following properties of II: (1) the enzyme has a high affinity for pyridoxal phosphate; (2) II can follow a decarboxylation-dependent transamination pathway forming apoenzyme as one of the products of this pathway; and (3) the phosphorylated adducts investigated readily bind to apo-II, but do not readily displace pyridoxal phosphate from holoenzyme. Incubation of holo-II with N-(5'-deoxypyridoxyl)-DL-DOPA, in the absence of added coenzyme, causes a rapid inactivation of enzyme (t1/2 = 5min) which is associated with a decrease in the coenzyme content of the enzyme. However, incubation of holoenzyme with the phosphorylated adduct, I, causes a much slower inactivation of enzyme (t1/2 = 30 min), whereas a short incubation (≤10 min) with either of the phosphorylated adducts increases the activity of holoenzyme. Calcns. indicate that the extent of reactivation of apoenzyme, formed via the decarboxylation-dependent transamination pathway, by excess exogenous coenzyme cannot be accounted for solely by reconstitution of holoenzyme. It is proposed that II has either a 2nd active site which has a low affinity for pyridoxal phosphate or a site(s) which, when occupied by pyridoxal phosphate, leads to an increase in the activity of the enzyme.

AN 1982:2806 CAPLUS Full-text

DN 96:2806

OREF 96:507a,510a

TI Inhibition of aromatic L-amino acid decarboxylase by coenzyme-amino acid adducts

AU Rudd, Edwin A.; Thanassi, John W.

CS Coll. Med., Univ. Vermont, Burlington, VT, 05405, USA

SO Biochemistry (1981), 20(26), 7469-75 CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

IT 79950-80-4

RL: BIOL (Biological study)

(aromatic amino acid decarboxylase inhibition by, kinetics of)

RN 79950-80-4 CAPLUS

CN L-Tyrosine, 3-hydroxy-N-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-

pyridinyl]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.

## OSC.G 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L10 ANSWER 32 OF 33 CAPLUS COPYRIGHT 2010 ACS on STN

AB The interaction between pyridoxyl amino acids and pig kidney decarboxylase was studied. Reactivation of the apoenzyme i.e. recombination of apo- and coenzymes in the presence of pyridoxal phosphate was very rapid but not immediate and the determination of inhibition consts. for the various pyridoxyl derivs. was difficult. The percent inhibition for 2 + 10-5M concns. of the following phosphopyridoxyl amino acids were: tyrosine 77, phenylalanine 66, methylamine 0, tyramine 40, and tyrosinol (0.7 + 10-5M) <5. The results show that for dopa-decarboxylases the phosphopyridyl derivs. are effective inhibitors of coenzyme-apoenzyme recombination and thus possess an affinity for the enzyme active site. Absence of the CO2H group as in tyramine or of the amino acid moiety as with methylamine reduces or annuls the inhibitory action. The results agree with those obtained with bacterial decarboxylase except in the case of the tyrosinol compound which is inhibited by the bacterial enzyme but not by the mammalian enzyme.

AN 1972:137410 CAPLUS Full-text

DN 76:137410

OREF 76:22279a,22282a

TI Inhibition of the apoenzyme of Dopa decarboxylase by phosphopyridoxyl-amino acids

AU Borri-Voltattorni, C.; Minelli, A.; Turano, C.

CS Fac. Farm., Univ. Perugia, Perugia, Italy

SO Bollettino - Societa Italiana di Biologia Sperimentale (1971), 47(21), 700-2

CODEN: BSIBAC; ISSN: 0037-8771

DT Journal

LA Italian

IT 36093-69-3

RL: BIOL (Biological study)

(dopa decarboxylase apoenzyme inhibition by)

RN 36093-69-3 CAPLUS

CN L-Tyrosine, N-[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]carbonyl]- (CA INDEX NAME)

L10 ANSWER 33 OF 33 CAPLUS COPYRIGHT 2010 ACS on STN

AB Thermodynamic parameters  $\Delta F^{\circ}37$ ,

 $\Delta \text{H}^{\circ}, \Delta \text{S}^{\circ}$ , and  $\Delta ^{\circ}$  p for

5'-phosphopyridoxyl-and pyridoxyl amino acid (aspartate, tyrosine)-apoenzyme complex formations are tabulated. Compensation phenomena may be of primary importance for catalytic mechanism of enzymes and may also play a role in the maintenance of a nearly constant level of enzymic activity under relatively large variations of pH values.

AN 1972:96331 CAPLUS Full-text

DN 76:96331

OREF 76:15505a,15508a

- TI Thermodynamic parameters for substrate-coenzyme-protein complex formation in B6-dependent enzymes
- AU Turano, C.; Borri Voltattorni, C.; Orlacchio, A.; Giartosio, A.
- CS Inst. Biol. Chem., Univ. Perugia, Perugia, Italy
- SO Eur. Biophys. Congr., Proc., 1st (1971), Volume 1, 45-8. Editor(s): Broda, E. Publisher: Verlag Wiener Med. Akad., Vienna, Austria. CODEN: 24KMAA
- DT Conference
- LA English
- IT 35930-97-3

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with pyridoxal phosphate-dependent enzymes)

RN 35930-97-3 CAPLUS

CN L-Phenylalanine, N-[[4-(hydroxymethyl)-6-methyl-5-(phosphonooxy)-3-pyridinyl]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.

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http://www.cas.org/support/stngen/stndoc/properties.html

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N 3 5 9 10 11 13 13 15 S



chain nodes : 7 8 9 10 11 19 20 21 22 ring nodes :

1 2 3 4 5 6 12 13 14 15 16 17

chain bonds :

 $7-8 \quad 7-9 \quad 9-10 \quad 10-11 \quad 11-12 \quad 19-20 \quad 19-21 \quad 19-22 \quad 19-26 \quad 26-27$ 

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16 \quad 16-17$ 

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-9 9-10 26-27

exact bonds :

10-11 11-12 19-26

normalized bonds :

12-13 12-17 13-14 14-15 15-16 16-17 19-20 19-21 19-22

isolated ring systems :

containing 1 :

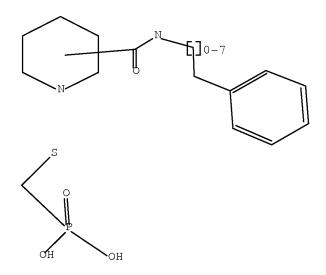
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FULL SCREEN SEARCH COMPLETED - 152 TO ITERATE

100.0% PROCESSED 152 ITERATIONS 145 ANSWERS

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L13 145 SEA SSS FUL L11

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28 L13 NOT L3

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=> s 113 not 13

=> d abs bib

L15 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN GI

The invention relates to phosphonic acid derivs. R1-X1-P(0) (X2-R2)-Y-Z-W1(A1-R3) (A2-R4)-W2(A3-R5) (A4-R6)-W3(A5-R7) (A6-R8)- A7-Q(T)-V(U)-A8-CR9R10-A9-R11 [R1, R2 are independently H or phospho-protecting groups; X1, X2 are independently O, S or NR12; Z is O, S, NR13 or CR4R5; A1-A9 are independently null, O, S, NR16, SO, SO2, CO, C(S), NR17CO, NR18C(S), NR19CONR2O, NR21C(S)NR22, NR23S(O), NR24SO2 or NR25CO2; Y is O or CR26R27; Q, V are independently CR28 or N; W1, W2, W3 are independently C or N; R3-R28, T, U are independently null, H, halo, (un)substituted alkyl, cycloalkyl, heterocyclyl, aryl, heteroaryl, etc.; or T and U may be connected by a single or double bond] and to pharmaceutical compns. containing the compds. for the treatment of diseases involving abnormal or undesired cell proliferation or mitosis. Thus, peptide phosphonic acid derivative I, prepared via peptide coupling in the solid phase, was a potent rotamase inhibitor (IC50 < 1  $\mu$ M).

AN 2005:612099 CAPLUS Full-text

DN 143:133696

TI Preparation of peptide phosphonic acid derivatives for the inhibition of undesired cell proliferation

IN Knolle, Jochen; Schutkowski, Mike; Hummel, Gerd; Tradler, Thomas; Jobron, Laurence; Christner, Claudia; Gibson, Christoph; Zischinsky, Gunther

PA Jerini A.-G., Germany

SO PCT Int. Appl., 110 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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			RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,		
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	WO	2004-EP14460				W		2004	1218											

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